

# Explicit form of the Bayesian posterior estimate of a quantum state under the uninformative prior

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**Abstract.** An analytical solution for the posterior estimate in Bayesian tomography of the unknown quantum state of an arbitrary quantum system (with a finite-dimensional Hilbert space) is found. First, we derive the Bayesian estimate for a pure quantum state measured by a set of arbitrary rank-1 POVMs under the uninformative (i.e. the unitary invariant or Haar) prior. The expression for the estimate involves the matrix permanents of the Gram matrices with repeated rows and columns, with the matrix elements being the scalar products of vectors giving the measurement outcomes. Second, an unknown mixed state is treated by the Hilbert-Schmidt purification. In this case, under the uninformative prior for the combined pure state, the posterior estimate of the mixed state of the system is expressed through the matrix  $\alpha$ -permanents of the Gram matrices of scalar products of vectors giving the measurement outcomes. In the mixed case, there is also a free integer parameter – the Schmidt number – which can be used to optimise the Bayesian reconstruction (for instance, in case of Schmidt number being equal to 1, the mixed state estimates reduces to the pure state estimate). We also discuss the perspectives of approximate numerical computation and asymptotic analytical evaluation of the Bayesian estimate using the derived formula.

## 1. Introduction

The purpose of the Quantum Tomography (QT) is reconstruction of the quantum state from the results of measurements [1]. The first QT experiments were performed in the early 1990-es [2, 4, 3, 5]. Nowadays, most of the tomographic reconstructions are performed by using the Maximum likelihood estimation (MLE) method proposed in Ref. [6] (see also Refs. [7, 8, 9, 10] for further and recent developments). In the MLE method one finds an estimate by maximising the likelihood function, the product of the conditional probabilities of measurement outcomes given by the Born rule. The MLE estimate is but a point estimate in the Hilbert space, nevertheless, it can be supplemented by the maximum-likelihood region, i.e. the region of largest likelihood among all regions of the same size [11] (for a similar approach of confidence regions in QT see Ref. [12]). On the other hand, the Bayesian approach in QT accounts for the available prior information on the unknown state by integrating the likelihood function with some prior probability distribution. It was pioneered in Ref. [13], where the unitary invariant prior (Haar measure) was used and the isotropic measurement scheme was shown to asymptotically saturate a bound on the extractable information.

In theory, convergence of the likelihood function to the Dirac distribution in the limit of large number of measurements (see, for instance, Refs. [14, 15]) causes an effective decoupling of the posterior probabilities from the prior information and the agreement between the MLE and Bayesian estimates (in accordance with the Bernstein - von Mises theorem [16]). In practice, Bayesian approach avoids many pitfalls of the MLE and is generally believed to be superior to the latter (see, for instance, Ref. [17]). However, the price to pay for the superiority is a higher computational complexity of the Bayesian QT as compared to the MLE method (another subtle point is the choice of prior, see for general discussion Ref. [18]). A systematic, moreover analytic, analysis of Bayesian QT for systems of 1/2-spins was carried out in Ref. [15], where the explicit formulae for the Bayesian estimates of pure as well as mixed quantum states were derived for various particular measurement schemes. Though there was no general analytical expression, a table of posterior estimates was presented and growth of complexity of the formulae was noted. Numerical schemes are being proposed to beat the sheer complexity of the Bayesian QT, for instance based on the advanced Monte Carlo methods [19]. For small systems (e.g. a qubit) it was theoretically and experimentally demonstrated [20, 21] that use of the adaptive Bayesian QT significantly improves the efficiency of reconstruction.

The purpose of the present work is to derive an explicit analytical formula for the Bayesian estimate of a quantum state under the uninformative prior. In the pure state estimation problem (i.e. when it is known that the unknown state is pure) the uninformative prior is the unitarily invariant (Haar) prior used already in Refs. [13, 15]. This is the prior which assigns equal probabilities to equal parts of the projective Hilbert space, i.e. all vectors of the Hilbert space are equally probable. In the case of a mixed unknown state there is no agreement on what prior should be considered as

the uninformative prior, since the mixed states form a convex set, not a space. However, similar as in Ref. [15], we make a physically relevant assumption that a mixed state is actually a part of the combined pure state of the system and an ancilla (i.e. we use the Hilbert-Schmidt purification), where we leave the dimension of the ancilla Hilbert space as an optimisation parameter. This simple trick allows one to introduce into the Bayesian estimate of the system state an effective dimension of the mixed system state. The effective dimension depends on the number of significantly nonzero eigenvalues in the unknown mixed state.

The paper is organized as follows. In section 2 we recall some basics of the Bayesian approach in QT and state our goal. In section 3 we derive an explicit formula for the Bayesian estimate of a pure quantum state. In section 4 we apply the result of section 3 to the unknown mixed state via the Hilbert-Schmidt purification with an ancilla system. In section 5 we review the available methods and insights on the numerical and analytical calculation of the matrix  $\alpha$ -permanents which are integral part of the derived analytical formulae. In section 6 we state the main results and problems for future research.

## 2. Bayesian quantum tomography with the uninformative prior

Consider the problem of reconstructing the state of a quantum system with  $d$ -dimensional Hilbert space  $H$ . Assume that the state is known to be pure<sup>‡</sup>. The Bayesian scheme starts with selecting a prior probability distribution, which we can cast in the form  $P(\psi)d\mu(\psi)$ , with  $d\mu(\psi)$  being the Haar (i.e. unitary invariant) measure in the Hilbert space, i.e.

$$d\mu(\psi) = (d-1)! \delta \left( \sum_{k=1}^d |\psi_k|^2 - 1 \right) \prod_{k=1}^d \frac{d\psi_k^* \wedge d\psi_k}{2i\pi} \quad (1)$$

where  $\psi_k$ ,  $k = 1, \dots, d$ , are projections of the state  $|\psi\rangle$  on some orthogonal basis in  $H$  and the Dirac distribution  $\delta(\dots)$  accounts for the normalization of the state (here the integration is in the complex plane of each  $\psi_k$ :  $d\psi_k^* \wedge d\psi_k / (2i\pi) = d\text{Re}(\psi_k) d\text{Im}(\psi_k) / \pi$ ). The Haar measure is normalized such that  $\int d\mu(\psi) = 1$ . The Haar prior, i.e.  $P(\psi) = 1$ , assigns equal probabilities to equal areas of the  $(2d-1)$ -dimensional hypersphere in the real projection of the complex  $d$ -dimensional space. In other words, all vectors in the Hilbert space are equally probable. Thus, if nothing is known about the true state of the system, except that it is pure, one would naturally set  $P(\psi) = 1$  (such prior was first used in Ref. [13]). One can rightfully call this prior uninformative.

An experimentalists is given an ensemble of systems which are prepared in the same pure state on which he/she performs measurements described by a Positive Operator Valued Measure (POVM) or by a set of POVMs (where an adaptive scheme can be implemented). We assume that all POVMs from the set have only elements of rank equal to 1<sup>§</sup> (but not the orthogonal projectors, in general). In the formulae below

<sup>‡</sup> The general case of a mixed state will be considered in a forthcoming work

<sup>§</sup> In the general case one can expand each POVM element in the basis of eigenvectors and use the below derived formulae.

the vectors from all POVMs enter symmetrically, thus it is convenient to use a single index for all elements from the set of POVMs. For instance, the resolution of unity (overcomplete for more than one POVM or single POVM with nonorthogonal elements) reads

$$\frac{1}{s} \sum_{k=1}^M |\phi_k\rangle\langle\phi_k| = I, \quad (2)$$

where  $M \geq d$  is the number of all possible outcomes  $|\phi_k\rangle$  from all measurements and  $s$  is the number of such rank-1 POVMs. Note that in general  $\langle\phi_k|\phi_l\rangle \neq 0$  for  $k \neq l$  and  $\langle\phi_k|\phi_k\rangle \neq 1$ .

Let us denote the observed frequency of the result  $|\phi_k\rangle$  to be  $n_k$  (for each particular POVM the respective frequencies sum to the number of measurements with that particular POVM). Let us denote the total number of measurements with all POVMs to be  $N$  (thus  $\sum_{k=1}^M n_k = N$ ). We will label the sequential outcomes of measurements by a Greek index, e.g.  $|\phi_{k_\alpha}\rangle$ , where  $1 \leq \alpha \leq N$  and  $1 \leq k_\alpha \leq M$ . The probability  $P(n_1, \dots, n_M|\psi)$  to obtain the frequencies  $n_1, \dots, n_M$  conditional on the state  $|\psi\rangle$  is given by the likelihood function<sup>||</sup> following from the Born rule:

$$P(n_1, \dots, n_M|\psi) = \prod_{\alpha=1}^N |\langle\phi_{k_\alpha}|\psi\rangle|^2 = \prod_{k=1}^M |\langle\phi_k|\psi\rangle|^{2n_k}. \quad (3)$$

The goal is to calculate the Bayesian estimate  $\rho$  (density matrix) on the system state given by the formula

$$\rho = \int d\mu(\psi) \frac{P(n_1, \dots, n_M|\psi)}{P(n_1, \dots, n_M)} |\psi\rangle\langle\psi|, \quad (4)$$

where the total probability of the outcomes,  $P(n_1, \dots, n_M)$ , reads

$$P(n_1, \dots, n_M) = \int d\mu(\psi) P(n_1, \dots, n_M|\psi). \quad (5)$$

### 3. Analytical formula for Bayesian estimate of a pure state

Eq. (4) involves integral over a polynomial in  $|\psi\rangle$  and  $\langle\psi|$  of order  $N$ . All such integrals can be easily evaluated by using the following identity

$$\int d\mu(\psi) (|\psi\rangle\langle\psi|)^{\otimes N} = \frac{S_N}{\text{Tr } S_N}, \quad S_N \equiv \frac{1}{N!} \sum_{\sigma} P_{\sigma}, \quad (6)$$

where  $S_N$  is the projector on the symmetric subspace of  $H^{\otimes N}$ , i.e. of the product of  $N$  system Hilbert spaces ( $P_{\sigma}$  is the unitary operator representation of permutation  $\sigma$  of the vectors from the individual spaces  $H$  in the tensor product belonging to  $H^{\otimes N}$ ). Indeed, trivially, the l.h.s. of Eq. (6) is an operator in the symmetric subspace  $H^{\otimes N}$ , moreover, it commutes with any permutation operator  $P_{\sigma}$ . Thus, it must be proportional to the identity operator in the symmetric subspace, i.e. to  $S_N$ . By taking the trace of both sides

<sup>||</sup> Since the order of the results is unimportant, one must use the multinomial factor at the likelihood function, but the factor cancels below due to normalization of the posterior distribution.

of Eq. (6) and using the Haar measure normalization one arrives at the denominator on the r.h.s., which is the number of basis states in  $H^{\otimes N}$ :  $\text{Tr } S_N = \frac{(N+d-1)!}{N!(d-1)!} \P$ . Now, Eq. (6) trivially leads to the following identity

$$\begin{aligned} \int d\mu(\psi) \prod_{\alpha=1}^N \langle x_\alpha | \psi \rangle \langle \psi | y_\alpha \rangle &= \frac{(\langle x_N | \cdots \langle x_1 |) S_N (|y_1 \rangle \cdots |y_N \rangle)}{\text{Tr } S_N} \\ &= \frac{(d-1)!}{(N+d-1)!} \text{per}(\mathcal{M}), \quad \mathcal{M}_{\alpha\beta} \equiv \langle x_\alpha | y_\beta \rangle. \end{aligned} \quad (7)$$

Here we have denoted by “per” the matrix permanent (see, for instance, Ref. [22]), which is defined for a  $N \times N$ -dimensional matrix  $A$  as follows

$$\text{per}(A) = \sum_{\sigma} \prod_{i=1}^N A_{i\sigma(i)}, \quad (8)$$

where the sum runs over all permutations  $\sigma$  of  $N$  column indices of  $A$ . Note that the matrix permanent is invariant under any permutation of rows (or columns) of  $A$ .

The identity (7) allows to evaluate the integral giving the Bayesian estimate (4). Indeed, we can take an element of  $\rho$  between two basis vectors from  $H$ , say  $\langle e_i | \rho | e_j \rangle$ , and use Eq. (7). We get

$$\rho = \frac{1}{N+d} \sum_{i,j=1}^d \frac{|e_i \rangle \text{per}(\mathcal{B}^{(i,j)}) \langle e_j|}{\text{per}(\mathcal{A})}, \quad (9)$$

where we have introduced two Gram matrices, a  $N \times N$ -dimensional matrix  $\mathcal{A}$  and a  $(N+1) \times (N+1)$ -dimensional matrix  $\mathcal{B}^{(i,j)}$ . They read

$$\mathcal{A}_{\alpha,\beta} = \langle \phi_{k_\alpha} | \phi_{k_\beta} \rangle, \quad \mathcal{B}^{(i,j)} = \begin{pmatrix} \mathcal{A} & V^{(j)} \\ [V^{(i)}]^\dagger & \delta_{i,j} \end{pmatrix}, \quad V_\alpha^{(l)} = \langle \phi_{k_\alpha} | e_l \rangle. \quad (10)$$

The expression on the r.h.s. of Eq. (9) can be simplified if we take into account two facts. First,  $\mathcal{A}$  is the matrix of repeated rows and columns of  $A_{lk} \equiv \langle \phi_l | \phi_k \rangle$ . Denoting by  $A[n_1, \dots, n_M | m_1, \dots, m_M]$  the matrix with the  $k$ -th row of  $A$  taken  $n_k$  times and the  $l$ -th column of  $A$  taken  $m_l$  times, we obtain  $\mathcal{A} = A[n_1, \dots, n_M | n_1, \dots, n_M]$  where  $n_k$  is the number of times the  $k$ -th result of measurement (i.e.  $|\phi_k\rangle$ ) has been registered. Similarly, the vector-column  $V^{(i)}$  consists of repeated scalar products, where each  $\langle e_i | \phi_k \rangle$  enters with the multiplicity  $n_k$ . By applying the Laplace expansion (see, for instance, Ref. [22]) to the matrix permanent of  $\mathcal{B}_{nm}$  twice, first with respect to the last column, then with respect to the last row, and using the repeated structure of the column-vector  $V^{(i)}$ , after some algebra (see details in Appendix A) we obtain from Eq. (9) the following expression for the posterior density matrix

$$\rho = \frac{1}{N+d} \left\{ I + \sum_{k,l=1}^M \frac{n_k n_l \text{per}(\mathcal{A}(l,k))}{\text{per}(\mathcal{A})} |\phi_k \rangle \langle \phi_l| \right\}, \quad (11)$$

where  $\mathcal{A}(l,k) \equiv A[n_1, \dots, n_l-1, \dots, n_M | n_1, \dots, n_k-1, \dots, n_M]$ , i.e. the  $(N-1) \times (N-1)$ -dimensional Gram matrix obtained from  $\mathcal{A}$  by crossing out one row of the scalar products

$\P$  One can also verify the identity (6) by direct integration in some basis.

with  $\langle \phi_l |$  and one column of the scalar products with  $|\phi_k\rangle$ . It is evident that the r.h.s. of Eq. (11) is invariant under rescaling of all the vectors by complex scalars  $|\phi_k\rangle \rightarrow \lambda_k |\phi_k\rangle$  (therefore, one can always consider the vectors to be normalized).

The denominator on the r.h.s. of Eq. (11) can be expanded by applying the Laplace formula (see Eq. (A.1) of Appendix A) to the matrix permanent and taking into account that matrix  $\mathcal{A}$  consists of repeated rows and columns. We have

$$\text{per}(\mathcal{A}) = \sum_{k=1}^M n_k \text{per}(\mathcal{A}(l|k)) \langle \phi_l | \phi_k \rangle = \frac{1}{N} \sum_{k,l=1}^M n_k n_l \text{per}(\mathcal{A}(l|k)) \langle \phi_l | \phi_k \rangle. \quad (12)$$

For instance, from Eq. (12) it is easy to see that the trace of the posterior density matrix is indeed equal to 1. Note that the posterior density matrix is such that it assigns *at least* the probability  $p(x) = 1/(N + d)$  to any outcome  $|x\rangle$  of future measurement, which is in accordance with what is generally expected on the basis of Laplace's rule of succession for  $d$  excluding outcomes [18] ( $|x\rangle$  and the orthogonal complement vectors from the standard basis) (see also Ref. [17]).

The fact that the matrix permanents appear in expression (7) and, hence, in formula (11) has a clear physical interpretation. Indeed, since our prior is uninformative, all vectors are equally probable before any measurement takes place. Therefore, the form of the total (i.e. unconditional) posterior probability of  $N$  measurement outcomes must be invariant with respect to simultaneous unitary transformation of all  $N$  vector outcomes (equivalent to unitary transformation of the pure system state on which we integrate with the Haar measure). The only scalars of a set of vectors are their scalar products. The only permutational invariant scalar (which is linear in each successive measurement outcome and its Hermitian conjugate, as the Born rule dictates) is the permanent of a Gram matrix of their scalar products, exactly as in Eq. (7).

Let us consider the special case of a qubit,  $d = 2$  (detailed analysis of this case was first carried out in Ref. [15], where growing complexity of the analytical formulae as  $N$  increases was noted). For any two vectors in the 2-dimensional Hilbert space we have

$$|\phi\rangle\langle\psi| = \frac{1}{2} \left\{ \langle\psi|\phi\rangle I + \sum_{j=1}^3 \langle\psi|\sigma_j|\phi\rangle \sigma_j \right\}, \quad (13)$$

where  $\sigma_j$ ,  $j = 1, 2, 3$ , are the Pauli matrices. Inserting Eq. (13) into the general expression for the posterior density matrix (11) and using expansion (12) to simplify the numerator we obtain the Bayesian estimate of the qubit pure state

$$\rho = \frac{1}{2} \left\{ I + \sum_{j=1}^3 v_j \sigma_j \right\}, \quad v_j \equiv \sum_{k,l=1}^M \frac{n_k n_l \text{per}(\mathcal{A}(l, k))}{(N + 2) \text{per}(\mathcal{A})} \langle \phi_l | \sigma_j | \phi_k \rangle. \quad (14)$$

Note that the vector  $\vec{v}$  is real as it should be.

Let us consider the simplest example of a von-Neumann POVM, i.e. a single POVM consisting of the orthogonal projectors,  $\langle \phi_l | \phi_k \rangle = \delta_{l,k}$ . In this special case we get

$$\text{per}(\mathcal{A}(l, k)) = \text{per}(\mathcal{A}(k, k)) \delta_{l,k}, \quad \text{per}(\mathcal{A}) = \prod_{k=1}^d n_k!.$$

Therefore Eq. (11) delivers in this case the expected result

$$\rho = \frac{1}{N+d} \left\{ I + \sum_{k=1}^d n_k |\phi_k\rangle\langle\phi_k| \right\} = \sum_{k=1}^d \frac{n_k+1}{N+d} |\phi_k\rangle\langle\phi_k|, \quad (15)$$

consistent with Laplace's rule of succession discussed above.

#### 4. Analytical formula for Bayesian estimate of a mixed state

Now let us consider the general case of a mixed state estimation. As discussed in the Introduction, we lift the unknown mixed state of the system to a pure state of the system (S) and an ancilla (A) by the Hilbert-Schmidt purification, i.e.

$$\rho^{(S)} = \text{Tr}_A \{ |\Psi^{(SA)}\rangle\langle\Psi^{(SA)}| \}, \quad (16)$$

where we denote  $d_S$  and  $d_A$  the dimensions of the Hilbert space of the system and the ancilla. Any density matrix of the system can be represented in the form (16) where  $d_A \leq d_S$  and coincides with the number of nonzero eigenvalues of  $\rho^{(S)}$ .

We consider the measurements performed only on the system, which, as before, are described by a set of rank-1 POVMs. We combine the outcomes of all measurements into a single set with one index, similar as in Eq. (2). In the combined Hilbert space each POVM element is given as

$$\Pi_k = |\phi_k\rangle\langle\phi_k| \otimes I_A = \sum_{j=1}^{d_A} |\phi_k\rangle\langle\phi_k| \otimes |a_j\rangle\langle a_j|, \quad (17)$$

where  $|a_j\rangle$ ,  $j = 1, \dots, d_A$  is some unspecified basis in the Hilbert space of the ancilla. In this formulation the total probability of  $N$  outcomes  $|\phi_{k_\alpha}\rangle$ ,  $\alpha = 1, \dots, N$ , where the outcome  $|\phi_k\rangle$  appears  $n_k$  times, is given by the following expression

$$P(n_1, \dots, n_M) = \sum_{j_1=1}^{d_A} \dots \sum_{j_N=1}^{d_A} \int d\mu(\Psi^{(SA)}) \prod_{\alpha=1}^N |\langle\phi_{k_\alpha}^{(S)}, a_{j_\alpha}^{(A)} | \Psi^{(SA)}\rangle|^2, \quad (18)$$

where  $\mu(\Psi^{(SA)})$  is the uninformative (i.e. the unitary invariant) prior in the combined Hilbert space, as in Eq. (1) and  $|\phi_k^{(S)}, a_j^{(A)}\rangle \equiv |\phi_k\rangle|a_j\rangle$ . Using expression (7) to evaluate the integral in Eq. (18) we obtain

$$P(n_1, \dots, n_M) = \sum_{j_1=1}^{d_A} \dots \sum_{j_N=1}^{d_A} \frac{(d_S d_A - 1)!}{(N + d_S d_A - 1)!} \text{per}(\mathcal{C}(j_1, \dots, j_N)), \quad (19)$$

where  $N \times N$ -dimensional matrix  $\mathcal{C}(j_1, \dots, j_N)$  is a tensor product of two Gram matrices:  $\mathcal{C}_{\alpha\beta}(j_1, \dots, j_N) = \langle\phi_{k_\alpha} | \phi_{k_\beta}\rangle \langle a_{j_\alpha} | a_{j_\beta}\rangle = \langle\phi_{k_\alpha} | \phi_{k_\beta}\rangle \delta_{j_\alpha, j_\beta}$ . The summation over the ancilla indices  $j_1, \dots, j_N$  in Eq. (19) can be carried out by using the following identity

$$\sum_{j_1=1}^{d_A} \dots \sum_{j_N=1}^{d_A} \prod_{\alpha=1}^N \delta_{j_\alpha, j_{\sigma(\alpha)}} = d_A^{\text{cyc}(\sigma)}, \quad (20)$$

where  $\text{cyc}(\sigma)$  is the number of disjoint cycles in the cycle decomposition of permutation  $\sigma$  (see, for instance, Ref. [23]). Here we have taken into account that by Eq. (8)

$\text{per}(\mathcal{C}(j_1, \dots, j_N))$  is the sum over all permutations  $\sigma$ , where each term has as a factor the product  $\prod_{\alpha=1}^N \delta_{j_\alpha, j_\sigma(\alpha)}$ , that each permutation can be uniquely represented as a product of disjoint cycles of the type  $j_{\alpha_1} \rightarrow j_{\alpha_2} \rightarrow \dots \rightarrow j_{\alpha_k} \rightarrow j_{\alpha_1}$ , and that (due to the delta-symbols) there is just one free index  $j$ , running from 1 to  $d_A$ , corresponding to each cycle. Using Eq. (20) into Eq. (19) we obtain the final expression for the total probability

$$P(n_1, \dots, n_M) = \frac{(d_S d_A - 1)!}{(N + d_S d_A - 1)!} \text{per}_{d_A}(\mathcal{A}), \quad (21)$$

where  $\mathcal{A}$  is a Gram matrix with repeated rows and columns, defined as before  $\mathcal{A} = A[n_1, \dots, n_M | n_1, \dots, n_M]$ , and  $\text{per}_\alpha(\dots)$  stands for the so-called  $\alpha$ -permanent (see, for instance, Refs. [24, 25, 26]) which is defined for any complex number  $\alpha$ . For a  $N \times N$ -dimensional matrix  $A$  it reads

$$\text{per}_\alpha(A) = \sum_{\sigma} \alpha^{\text{cyc}(\sigma)} \prod_{i=1}^N A_{i, \sigma(i)}, \quad (22)$$

where  $\text{cyc}(\sigma)$  is the number of disjoint cycles in the cycle decomposition of permutation  $\sigma$ . Note that the  $\alpha$ -permanent is also invariant but under the *simultaneous* permutation of rows and columns of the matrix (in fact, only such a permutational invariance follows from the obvious permutation invariance of the measurement results in the Likelihood function).

Now we apply a similar strategy to derive the Bayesian estimate of the unknown mixed state as we have used in the pure state estimation in the previous section, i.e. we consider the matrix element  $\langle n | \rho^{(S)} | m \rangle$  of the Bayesian estimate for a mixed state

$$\rho^{(S)} = \int d\mu(\Psi^{(SA)}) \frac{P(n_1, \dots, n_M | \Psi^{(SA)})}{P(n_1, \dots, n_M)} \text{Tr}_A \{ |\Psi^{(SA)}\rangle \langle \Psi^{(SA)}| \} \quad (23)$$

and use the result (21) for  $N+1$  vectors with  $\langle \phi_{N+1} | \equiv \langle n |$  and  $|\phi_{N+1}\rangle = |m\rangle$ . Using Eq. (21) into Eq. (23) we obtain (here  $|e_i\rangle$ ,  $i = 1, \dots, d_S$ , is a basis in the system Hilbert space)

$$\rho^{(S)} = \frac{1}{N + d_S d_A} \sum_{i,j=1}^{d_S} \frac{|e_i\rangle \text{per}_{d_A}(\mathcal{B}^{(i,j)}) \langle e_j|}{\text{per}_{d_A}(\mathcal{A})}, \quad (24)$$

where the matrix  $\mathcal{B}^{(n,m)}$  is defined in Eq. (10) of the previous section. Eq. (24) reduces to Eq. (9) for  $d_A = 1$ , i.e. when the system state is a pure state. Using the expansion similar to the Laplace's for the  $\alpha$ -permanent, as shown in Appendix B, the mixed state estimate (24) can be simplified to the following form

$$\rho^{(S)} = \frac{1}{N + d_S d_A} \left\{ d_A I_S + \frac{\sum_{k,l=1}^M n_k (n_l + [d_A - 1]^{\delta_{k,l}}) \text{per}_{d_A}(\mathcal{A}(l, k)) |\phi_k\rangle \langle \phi_l|}{\text{per}_{d_A}(\mathcal{A})} \right\}, \quad (25)$$

$\mathcal{A}(l, k) = A[n_1, \dots, n_l - 1, \dots, n_M | n_1, \dots, n_k - 1, \dots, n_M]$ , i.e. defined similar as in the pure case, and  $I_S$  is the identity operator in the system Hilbert space.

Expression (25) gives a valid density matrix (i.e. the r.h.s. is positive definite Hermitian operator of unit trace) for any positive integer value of  $d_A$  by derivation.



Moreover, the sum in the numerator in the second term in the parenthesis on the r.h.s. of Eq. (25) is a homogeneous polynomial of order at most  $N$  in  $d_A$ .

Let us compare the estimates for the pure and mixed states in the case of a single von-Neumann POVM. We have in this case by simple computation (similar as in Appendix B).

$$\text{per}_{d_A}(\mathcal{A}) = n_k d_A \text{per}_{d_A}(\mathcal{A}(k, k)). \quad (26)$$

Hence, by using the orthogonality of the POVM elements from Eqs. (26) and (24) we get

$$\rho^{(S)} = \frac{d_A}{N + d_S d_A} \left\{ I_S + \sum_{k=1}^M \frac{n_k}{d_A} |\phi_k\rangle\langle\phi_k| \right\} = \sum_{k=1}^M \frac{n_k + d_A}{N + d_S d_A} |\phi_k\rangle\langle\phi_k|. \quad (27)$$

Estimate (27) is again consistent with Laplace's rule of succession. Indeed, this is easily seen by reducing it to the pure state estimate (15) for the same POVM by rescaling the number of measurements as follows  $N' \equiv N/d_A$  and the frequencies as  $n'_k \equiv n_k/d_A$ . Thus, one can interpret the results of each run by a  $d_S d_A$ -sided die with each side having a number from 1 to  $d_S$  (represented by index  $k$  in Eq. (27)) and a color from a set of  $d_A$  colours appearing with equal probability independently of the numbers, where we only register the numbers.

## 5. Perspectives of numerical calculation of the Bayesian estimate by using the derived formula

Numerical evaluation of the  $\alpha$ -permanent, in general, is a daunting task. Indeed, it is known that calculation of the matrix permanent for a general matrix has the #P-complete level of the computational complexity [27]. The best known algorithm for the permanent of a general matrix is given by Ryser's method [28] which requires  $\mathcal{O}(N^2 2^N)$  flop operations for the  $N \times N$ -dimensional matrix.

However, this general complexity is significantly reduced by the fact that one has to compute the permanent of matrices with *repeated* rows and columns. Indeed, only such matrices appear in the Bayesian quantum tomography, since for large number of measurements  $N$ , one will eventually have repetitions of the measurement results, where, generally,  $n_k \gg 1$  for  $N \gg d_S$ . The expected complexity of the permanent for a matrix with bounded rank  $\leq R$  is  $\mathcal{O}(N^R)$  [30]. Moreover, there is a modified Ryser's algorithm having the number of necessary flops significantly reduced down to  $\mathcal{O}(N^M)$  for the case of a  $N \times N$ -dimensional matrix with repeated columns and/or rows, where  $M$  different columns are possible (see, for the details, Appendix D in Ref. [31]).

The Ryser's method and its modification apply to the usual matrix permanent. There is no known generalisation for the  $\alpha$ -permanent. The computational complexity of the latter is also not yet completely understood. However, it is conjectured that the  $\alpha$ -permanent has the same complexity as the usual permanent for any  $\alpha > 0$  [32] (note that for  $\alpha = -1$  the  $\alpha$ -permanent is the usual determinant modified by a sign factor).

There are reasons to believe that it is the same as of the usual matrix permanent if  $\alpha$  is a positive integer, as in our case.

Another, and perhaps more crucial, observation is that the exact values of the coefficients in the Bayesian estimate (24), expressed through the  $\alpha$ -permanents, are not needed. One only has to estimate the  $\alpha$ -permanents to an error of order  $\mathcal{O}(N^{-2})$ . Indeed, the zeroth order asymptotic estimate  $\sim \mathcal{O}(1)$  coincides with the usual Maximum Likelihood estimate due to the above discussed convergence of the two in the limit of large number of measurements (this can be established also directly by using the asymptotic approximation of the matrix permanent developed in Ref. [31]). Hence, for large number of measurements  $N \gg d_S$ , the first nontrivial contribution of the Bayesian approach is to give the estimation error for the Maximal Likelihood estimate, which would require computing the  $\mathcal{O}(N^{-1})$  term in the asymptotic approximation of the  $\alpha$ -permanent. Indeed, the Maximal Likelihood estimate has an error of the order at least  $\mathcal{O}(N^{-1})$  for large  $N \gg d_S$ , since this is the order of the minimal probability assigned to any outcome by Laplace's rule of succession. Such an error is given by the first-order term in the asymptotic expansion of the derived analytical formula for the Bayesian estimate. However, even for the usual permanent, such an asymptotic term is yet not known in the explicit form and one must resort to numerics. To date, an efficient method for computing the  $\alpha$ -permanent, similar as for the usual permanent (outlined in Appendix D in [31]) is still missing. Hopefully, since the  $\alpha$ -permanents have many other important applications in physics and mathematics (see, for instance, Refs. [24, 25, 26, 32]) such a method will be found.

## 6. Conclusion

We have derived the explicit formula for the Bayesian estimate of a mixed quantum state of an arbitrary system with a finite-dimensional Hilbert space, applicable for the uninformative prior distribution of the system state. The uninformative prior used here is defined as the Haar measure in the projected Hilbert space of a pure state. For a mixed system state, the Hilbert-Schmidt purification to a pure state of a system and an ancilla is used, which one of the possible physical interpretations of a mixed state. The explicit formula involves the well-known mathematical object: the matrix  $\alpha$ -permanent. The dimension of the Hilbert space of the ancilla system is equal to the number of nonzero eigenvalues of the system density matrix. It can be used for an adaptive determination of the effective dimension of the reconstructed density matrix. Perspectives of the numerical calculations based on the derived formulae are discussed, it is important that the matrix permanents appearing in the Bayesian QT are of the matrices with repeated rows and columns, for which there is significant reduction of the computational complexity of the matrix permanent (which is, in general, exponentially hard to compute). Moreover, the exact coefficients, given by the matrix permanents, are not required, only the first two terms in the asymptotic expansion in  $N$  (the number of all measurements) is needed for given the estimate itself and the error of

the reconstruction. Therefore, there is significant expectation that in near future one would develop a method, analytical or numerical, for such an approximate evaluation of the matrix  $\alpha$ -permanents, which would allow effective computation of the posterior estimate in the Bayesian QT. We leave this as a problem for future research.

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## Appendix A. Derivation of the formula for posterior density matrix in case of pure state estimation

We will use the column or row expansion formula for the matrix permanent (see, for instance, Ref. [22]). For  $N \times N$ -dimensional matrix  $A$  it reads

$$\text{per}(B) = \sum_{k=1}^N \text{per}(B(k, N)) B_{k, N}, \quad (\text{A.1})$$

where  $B(l, m)$  is the matrix obtained from matrix  $B$  by crossing out the  $l$ -th row and  $m$ -th column. Then, using the expansion of Eq. (A.1) for the last column (i.e. with respect to  $V^{(i)}$ ) in the matrix  $\mathcal{B}^{(i,j)}$  of Eq. (10) of section 2 we get

$$\text{per}(\mathcal{B}^{(i,j)}) = \text{per}(\mathcal{A}) \delta_{i,j} + \sum_{\alpha=1}^N \text{per}(\mathcal{B}^{(i,j)}(\alpha|N+1)) \langle \phi_{k_\alpha} | e_i \rangle. \quad (\text{A.2})$$

Now, using the expansion of Eq. (A.1) with respect to the last row in  $\mathcal{B}^{(i,j)}(\alpha|N+1)$  (i.e. with respect to  $\tilde{V}^{(j)}$ ) we obtain

$$\text{per}(\mathcal{B}^{(i,j)}(\alpha|N+1)) = \sum_{\beta=1}^N \text{per}(\mathcal{B}^{(i,j)}(\alpha, N+1|\beta, N+1)) \langle e_j | \phi_{k_\beta} \rangle. \quad (\text{A.3})$$

Finally, using that  $\mathcal{B}^{(i,j)}(\alpha, N+1|\beta, N+1) = \mathcal{A}(k_\alpha|k_\beta)$  in the notations of section 2 and inserting the r.h.s. of Eq. (A.3) into Eq. (A.2), using that each vector-row  $\langle \phi_l |$  (vector-column  $|\phi_k\rangle$ ) appears exactly  $n_l$  ( $n_k$ ) times in the summation over  $\alpha$  ( $\beta$ ), whereas the coefficient is  $\text{per}(\mathcal{A}(l|k)) \langle e_j | \phi_k \rangle \langle \phi_l | e_i \rangle$ , we obtain the expression on the r.h.s. of Eq. (11) of section 2.

## Appendix B. Derivation of the formula for posterior density matrix in case of mixed state estimation

The derivation is based on the expansion for the  $\alpha$ -permanent, similar to the Laplace expansion. The  $d_A$ -permanent of  $\mathcal{B}^{(i,j)}$  is by definition (10)

$$\text{per}_{d_A}(\mathcal{B}^{(i,j)}) = \sum_{\sigma} \prod_{\alpha=1}^{N+1} d_A^{cyc(\sigma)} \langle \varphi_{k_\alpha} | \tilde{\varphi}_{k_{\sigma(\alpha)}} \rangle, \quad (\text{B.1})$$

where  $|\varphi_{k_\alpha}\rangle = |\tilde{\varphi}_{k_\alpha}\rangle = |\phi_{k_\alpha}\rangle$ ,  $\alpha = 1, \dots, N$  and  $|\varphi_{k_{N+1}}\rangle = |i\rangle$  and  $|\tilde{\varphi}_{k_{N+1}}\rangle = |j\rangle$ . Now, as compared to the similar expansion in Eq. (A.1)-(A.2) for the usual permanent, we need to check how the number of cycles decomposes for a decomposition of the permutation  $\sigma$  over  $N+1$  elements into a transposition of  $\alpha$ -th and  $(N+1)$ -th elements,  $(\alpha, N+1)$ , and a permutation  $\sigma'$  of the first  $N$  elements, i.e.

$$\sigma = \sigma' \cdot (\alpha, N+1). \quad (\text{B.2})$$

Obviously, if  $\alpha = N+1$  (the  $N+1$ -th element is left in place by  $\sigma$ ) then  $\text{cyc}(\sigma) = \text{cyc}(\sigma') + 1$ , since there is one additional 1-cycle (fixed point  $N+1$ ) in permutation  $\sigma$  as compared to the cycle decomposition of  $\sigma'$ . Otherwise,  $\alpha \neq N+1$ , both permutations have the same number of cycles, since now  $(N+1)$ -th element belongs to some cycle of  $\sigma'$ . Thus we obtain a formula for the decomposition as in Eq. (B.2)

$$\text{cyc}(\sigma' \cdot (\alpha, N+1)) = \text{cyc}(\sigma') + \delta_{\alpha, N+1}. \quad (\text{B.3})$$

Using the result (B.3) and similar expansion steps as in the derivation of E. (A.3) we obtain:

$$\begin{aligned} \text{per}_{d_A}(\mathcal{B}^{(i,j)}) &= \text{per}_{d_A}(\mathcal{A})d_A\delta_{i,j} + \sum_{\alpha=1}^N \text{per}_{d_A}(\mathcal{B}^{(i,j)}(\alpha|N+1)) \langle \phi_{k_\alpha} | e_j \rangle \\ &= \text{per}_{d_A}(\mathcal{A})d_A\delta_{i,j} + \sum_{\alpha,\beta=1}^N d_A^{\delta_{\alpha,\beta}} \text{per}_{d_A}(\mathcal{B}^{(i,j)}(\alpha, N+1|\beta, N+1)) \langle e_i | \phi_{k_\beta} \rangle \langle \phi_{k_\alpha} | e_j \rangle. \end{aligned} \quad (\text{B.4})$$

Therefore, we have

$$\rho^{(S)} = \frac{1}{N + d_S d_A} \left\{ d_A I_S + \frac{\sum_{\alpha,\beta=1}^N d_A^{\delta_{\alpha,\beta}} \text{per}_{d_A}(\mathcal{B}^{(i,j)}(\alpha, N+1|\beta, N+1)) |\phi_{k_\beta}\rangle \langle \phi_{k_\alpha}|}{\text{per}_{d_A}(\mathcal{A})} \right\},$$

where we have used the permutational invariance of the  $\alpha$ -permanent with respect to simultaneous permutation of rows and columns. Now, counting the number of equal terms in the numerator and using that for  $|\phi_{k_\beta}\rangle = |\phi_k\rangle$  and  $|\phi_{k_\alpha}\rangle = |\phi_l\rangle$  we have  $\text{per}_{d_A}(\mathcal{B}^{(i,j)}(\alpha, N+1|\beta, N+1)) = \text{per}_{d_A}(\mathcal{A}(l, k))$ , we obtain the resulting expression in the form of Eq. (24).

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